Table SI-1. Characterization of β-sheet geometry in amicyanin Δ is the difference between the α-carbon to α-carbon distance in the n^{th} extended and the α-carbon distance to α-carbon distance in the native state

A. Ladder 1: residues 42 to 47 bonded to residues 76 to 81

β-paired residues	**H bond (Å) native state**	**α-carbon distance (Å) native state**	**α-carbon distance (Å) n^{th} extended state**		**Δ(Å)**
THR 42 to THR 81	2.744	3.961	1	5.658	1.70
			2	5.983	2.02
			3	6.166	2.21
			4	6.724	2.76
			5	6.400	2.44
			6	6.235	2.27
VAL 43 to LEU 80	2.815	5.509	1	7.889	2.38
			2	8.331	2.82
			3	8.766	3.26
			4	8.744	3.24
			5	8.901	3.39
			6	8.460	2.95
THR 44 to SER 79	2.769	4.187	1	5.997	1.81
			2	6.308	2.12
			3	6.692	2.51
			4	6.838	2.65
			5	6.769	2.58
			6	6.391	2.20
TRP 45 to TYR 78	2.910	5.495	1	7.865	2.37
			2	8.299	2.8
			3	8.656	3.16
			4	8.608	3.11
			5	8.554	3.06
			6	8.326	2.83
ILE 46 to ALA 77	---	4.274	1	6.125	1.85
			2	6.318	2.04
			3	6.282	2.01
			4	6.039	1.77
			5	6.354	2.08
			6	6.129	1.86

ASN 47 to GLN 76	2.934	5.742	1	7.878	2.14
			2	7.048	1.31
			3	6.169	0.43
			4	7.378	1.64
			5	7.255	1.51
			6	6.794	1.05

B. Ladder 2: residues 42 to 47 bonded to residues 21 to 25

β-paired residues	H bond (Å) native state	α-carbon distance (Å) native state	α-carbon distance (Å) n^{th} extended state		Δ(Å)
THR 44 to ILE 21	2.843	5.937	1	7.915	1.98
			2	8.196	2.26
			3	6.918	0.98
			4	6.661	0.72
			5	7.779	1.84
			6	8.086	2.15
THR 44 to VAL 23	2.897	6.259	1	8.994	2.74
			2	9.487	3.23
			3	10.080	3.82
			4	10.270	4.01
			5	10.580	4.32
			6	10.540	4.28
TRP 45 to VAL 22	---	5.674	1	7.968	2.29
			2	7.891	2.22
			3	8.527	2.85
			4	7.698	2.02
			5	7.461	1.79
			6	7.307	1.63
ILE 46 to VAL 23	2.963	6.367	1	9.068	2.70
			2	8.196	1.83
			3	6.918	0.55
			4	6.661	0.29
			5	7.779	1.41
			6	8.086	1.72
ILE 46 to ILE 25	2.872	6.057	1	8.735	2.68
			2	9.258	3.20
			3	10.110	4.05
			4	10.620	4.56
			5	10.350	4.29
			6	9.724	3.67

ASN 47 to ASP 24	---	6.128	1	8.807	2.68
			2	9.218	3.09
			3	9.699	3.56
			4	9.243	3.12
			5	9.229	3.10
			6	8.387	2.26

C. Ladder 1 and Ladder 2 residues bonded to other residues

β-paired residues	H bond (Å) native state	α-carbon distance (Å) native state	α-carbon distance (Å) n^{th} extended state		Δ(Å)
TRP 45 to TYR 90	3.053	12.11	1	17.35	5.24
			2	18.22	6.11
			3	19.36	7.25
			4	19.49	7.38
			5	19.62	7.51
			6	18.90	6.79
ASN 47 to GLU 49	3.076	5.694	1	7.519	1.83
			2	7.552	1.86
			3	8.034	2.34
			4	7.724	2.03
			5	7.848	2.15
			6	7.520	1.83
ASN 47 to MET 51	2.983	8.456	1	11.65	3.19
			2	11.86	3.4
			3	12.27	3.81
			4	12.02	3.56
			5	12.25	3.79
			6	11.87	3.41
ASN 47 to MET 72	2.929	6.245	1	8.930	2.69
			2	8.961	2.72
			3	9.198	2.95
			4	8.828	2.58
			5	9.020	2.78
			6	8.826	2.58
ASN 47 to GLU 75	2.761	5.360	1	4.221	-1.14
			2	4.200	-1.16
			3	4.155	-1.21
			4	3.559	-1.80
			5	4.086	-1.27
			6	5.099	-0.26

GLN 76 to LYS 73	3.133	5.559	1	7.847	2.29
	2.984		2	8.207	2.65
			3	7.912	2.35
			4	9.241	3.68
			5	8.912	3.35
			6	7.861	2.3

ALA 77 to PHE 11	2.989	5.279	1	7.409	2.13
	2.721		2	7.470	2.19
			3	4.938	-0.34
			4	4.749	-0.53
			5	5.348	0.07
			6	6.324	1.05

THR 81 to THR 4	2.886	5.237	1	7.481	2.24
	2.963		2	7.608	2.37
			3		---
			4		---
			5		---
			6		---

D. Ladder 3: residues 86 to 92 bonded to residues 95 to 104

β-paired residues	H bond (Å) native state	α-carbon distance (Å) native state	α-carbon distance (Å) n^{th} extended state		Δ(Å)
GLY 86 to VAL 104	2.920	5.286	1	---	---
	2.831		2	---	---
			3	---	---
			4	---	---
			5	---	---
			6	---	---
THR 87 to VAL 103	---	4.409	1	6.253	1.84
			2	---	---
			3	---	---
			4	---	---
			5	---	---
			6	---	---
TYR 88 to VAL 102	2.894	5.241	1	7.519	2.28
	2.929		2	7.776	2.54
			3	---	---
			4	---	---
			5	---	---
			6	---	---
TYR 88 to GLU 84	2.776	10.324	1	10.85	0.53
			2	11.03	0.71
			3	8.615	-1.71
			4	10.13	-0.19
			5	9.201	-1.12
			6	9.391	-0.93
ASP 89 to LYS 101	2.922	4.198	1	6.010	1.81
			2	---	---
			3	---	---
			4	---	---
			5	---	---
			6	---	---

TYR 90 to GLY 100	2.938	5.479	1	7.829	2.35
	3.017		2	8.253	2.77
			3	8.622	3.14
			4	8.760	3.28
			5	---	---
			6	---	---

HIS 91 to ARG 99	---	4.339	1	6.232	1.89
			2	6.221	1.88
			3	6.708	2.37
			4	6.891	2.55
			5	6.934	2.60
			6	---	---

CYS 92 to MET 98	3.175	5.648	1	7.625	1.98
			2	7.939	2.29
			3	8.294	2.65
			4	8.299	2.65
			5	8.276	2.63
			6	8.067	2.42

HIS 95 to MET 98	2.902	5.846	1	7.781	1.94
			2	8.144	2.30
			3	9.770	3.92
			4	9.337	3.49
			5	10.68	4.83
			6	9.844	4.00

HIS 95 to CYS 92	3.073	5.159	1	7.056	1.90
	3.444		2	5.850	0.69
			3	6.360	1.20
			4	6.491	1.33
			5	8.026	2.87
			6	7.006	1.85

PRO 96 to ARG 99	2.708	6.781	1	9.623	2.84
	3.203		2	9.648	2.87
			3	10.79	4.01
			4	11.46	4.68
			5	11.93	5.15
			6	---	---

E. Ladder 3 residues bonded to other residues

β-paired residues	H bond (Å) native state	α-carbon distance (Å) native state	α-carbon distance (Å) n^{th} extended state		Δ(Å)
TYR 90 to **TRP 45**	3.053	12.11	1	17.35	5.24
			2	18.22	6.11
			3	19.36	7.25
			4	19.41	7.30
			5	19.62	7.51
			6	18.90	6.79
HIS 91 to HIS 56	2.961	5.302	1	7.620	2.32
			2	7.830	2.53
			3	8.454	3.15
			4	8.374	3.07
			5	8.538	3.24
			6	8.546	3.24
CYS 92 to HIS 53	3.773	6.152	1	8.737	2.59
			2	8.743	2.59
			3	8.701	2.55
			4	9.028	2.88
			5	9.259	3.11
			6	8.857	2.71
CYS 92 to ASN 54	3.926	5.313	1	7.516	2.20
	3.640		2	7.836	2.52
			3	8.185	2.87
			4	8.279	2.97
			5	8.420	3.11
			6	7.765	2.45
HIS 95 to HIS 53	3.144	7.840	1	10.740	2.90
			2	7.518	-0.32
			3	5.109	-2.73
			4	5.677	-2.16
			5	3.905	-3.94
			6	4.459	-3.39

LYS 101 to PRO 33	2.810	6.090	1	8.985	2.90
			2	9.407	3.32
			3	9.898	3.81
			4	---	---
			5	---	---
			6	---	---

LYS 101 to LEU 35	3.124	6.498	1	9.275	2.78
			2	8.827	2.33
			3	9.688	3.19
			4	---	---
			5	---	---
			6	---	---

LYS 101 to ASP 89	2.922	4.198	1	6.010	1.81
			2	6.350	2.15
			3	6.654	2.46
			4	---	---
			5	---	---
			6	---	---

VAL 103 to LEU 35	2.790	6.075	1	8.728	2.65
			2	---	---
			3	---	---
			4	---	---
			5	---	---
			6	---	---

VAL 103 to VAL 37	2.899	6.298	1	8.787	2.49
			2	---	---
			3	---	---
			4	---	---
			5	---	---
			6	---	---

Figure SI-1A

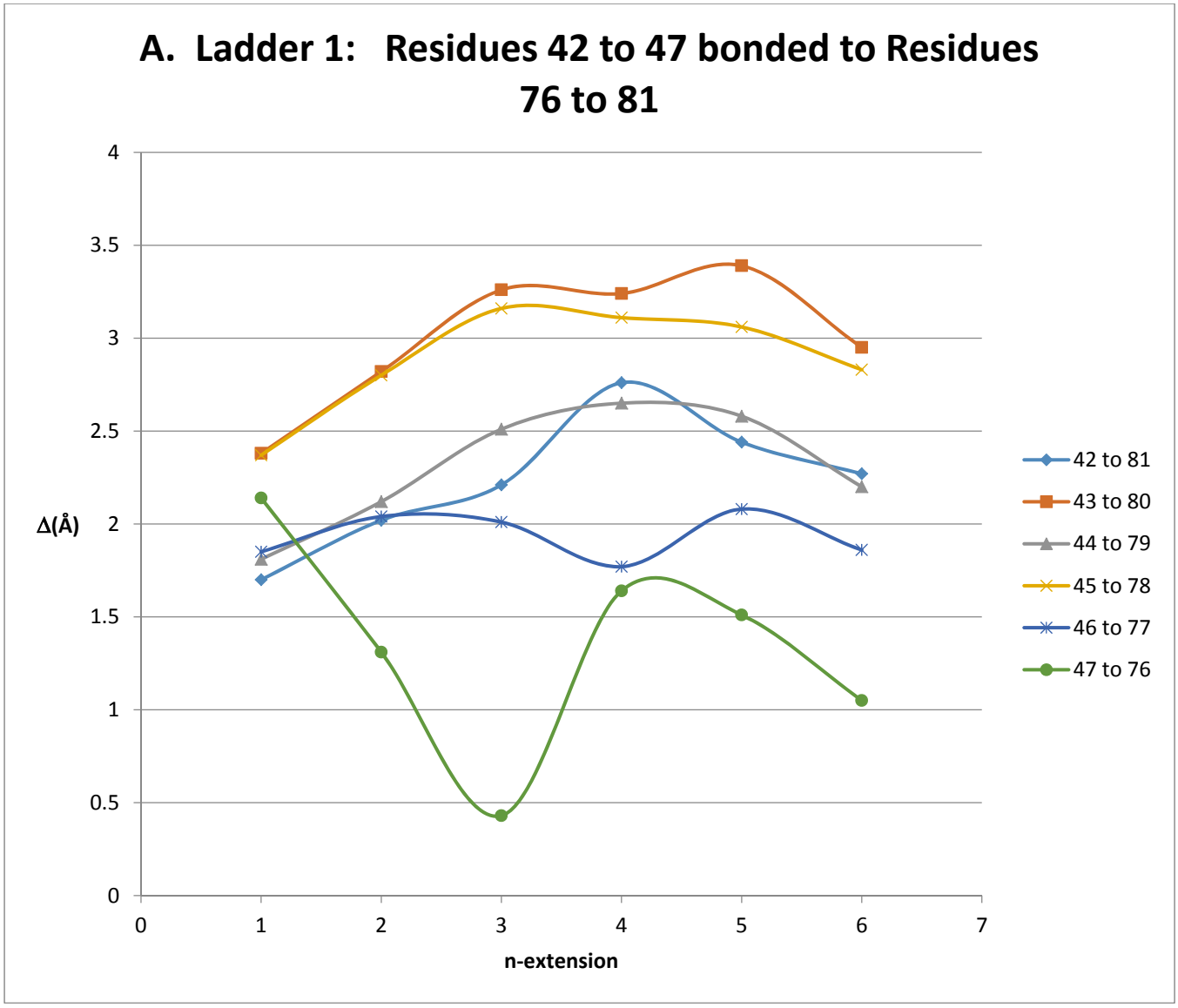

A. Ladder 1: Residues 42 to 47 bonded to Residues 76 to 81
Δ(Å)
n-extension
0
0.5
1
1.5
2
2.5
3
3.5
4
0
1
2
3
4
5
6
7
42 to 81
43 to 80
44 to 79
45 to 78
46 to 77
47 to 76

Figure SI-2A

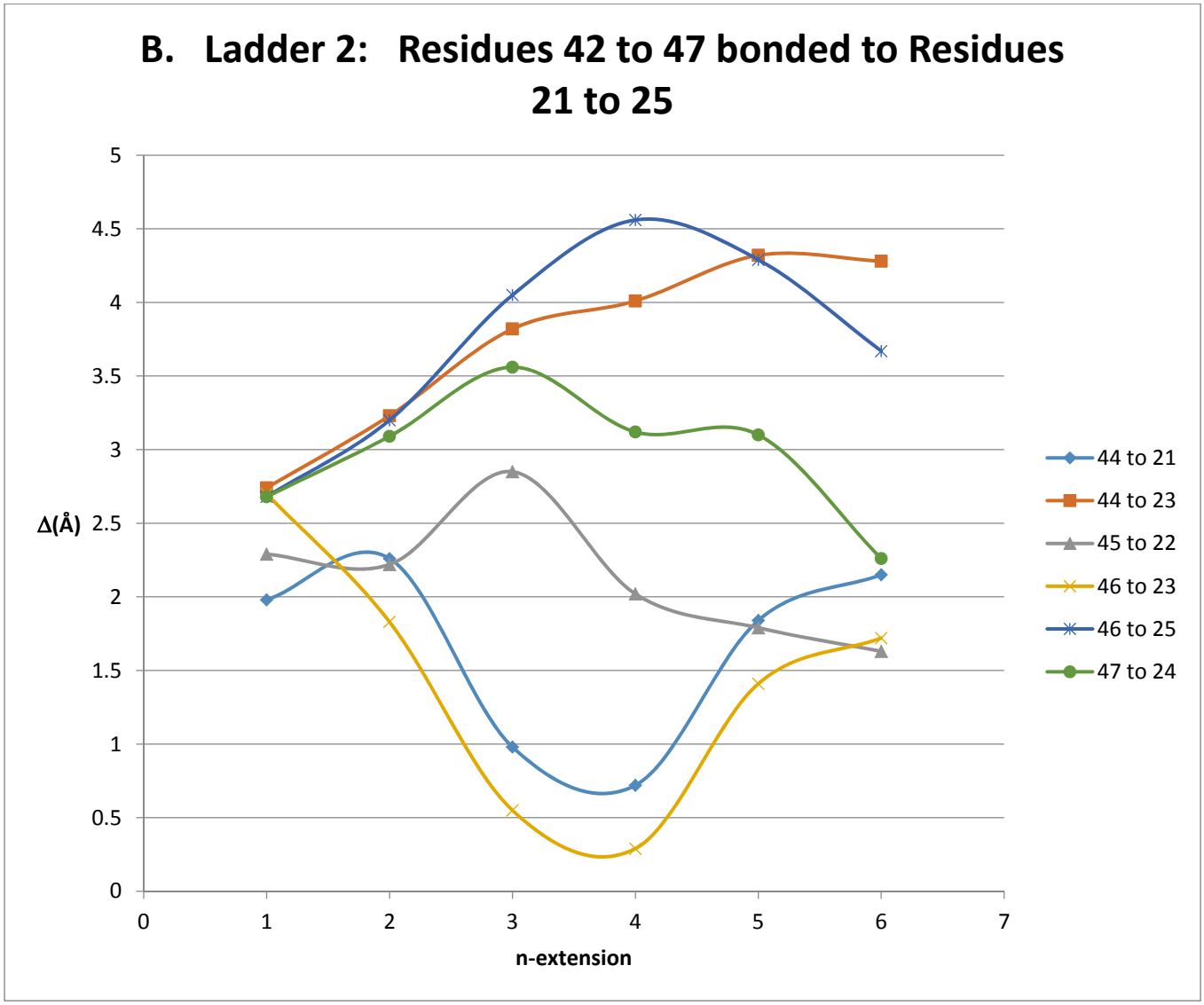

B. Ladder 2: Residues 42 to 47 bonded to Residues 21 to 25
Δ(Å)
n-extension
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
1
2
3
4
5
6
7
44 to 21
44 to 23
45 to 22
46 to 23
46 to 25
47 to 24

Figure SI-3A

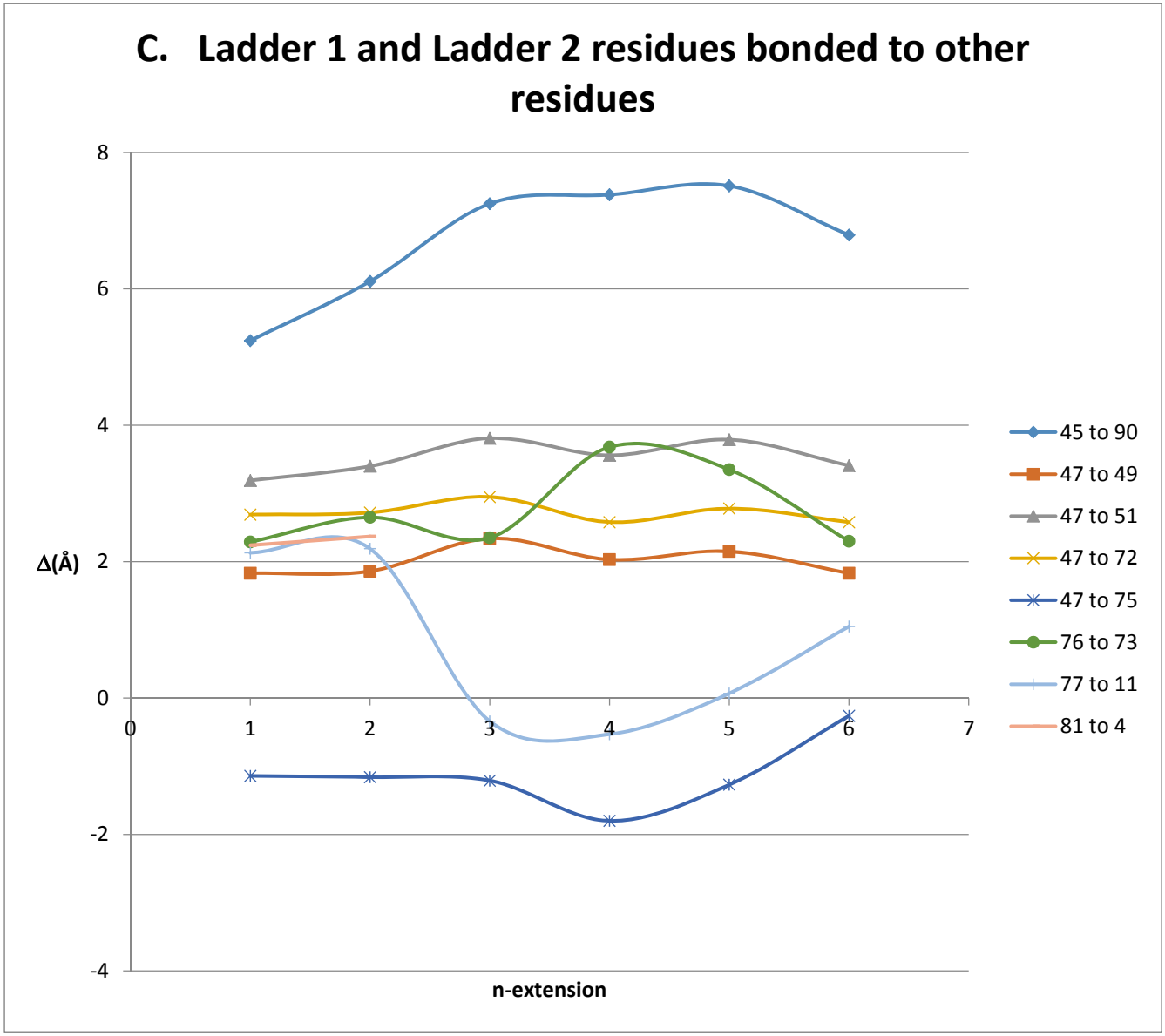

C. Ladder 1 and Ladder 2 residues bonded to other residues
8
6
4
2
0
-2
-4
Δ(Å)
0
1
2
3
4
5
6
7
n-extension
45 to 90
47 to 49
47 to 51
47 to 72
47 to 75
76 to 73
77 to 11
81 to 4

Figure SI-4A

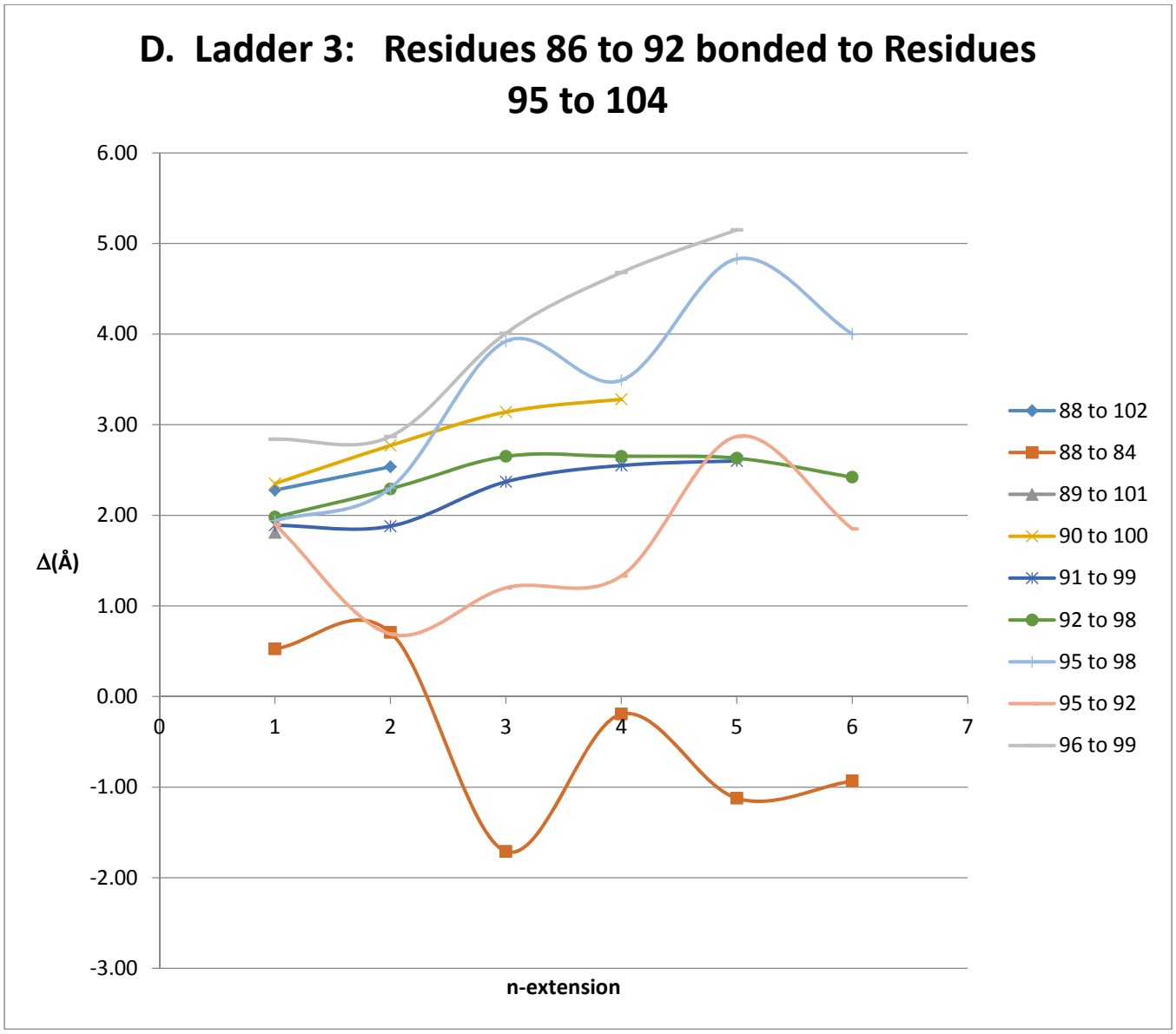
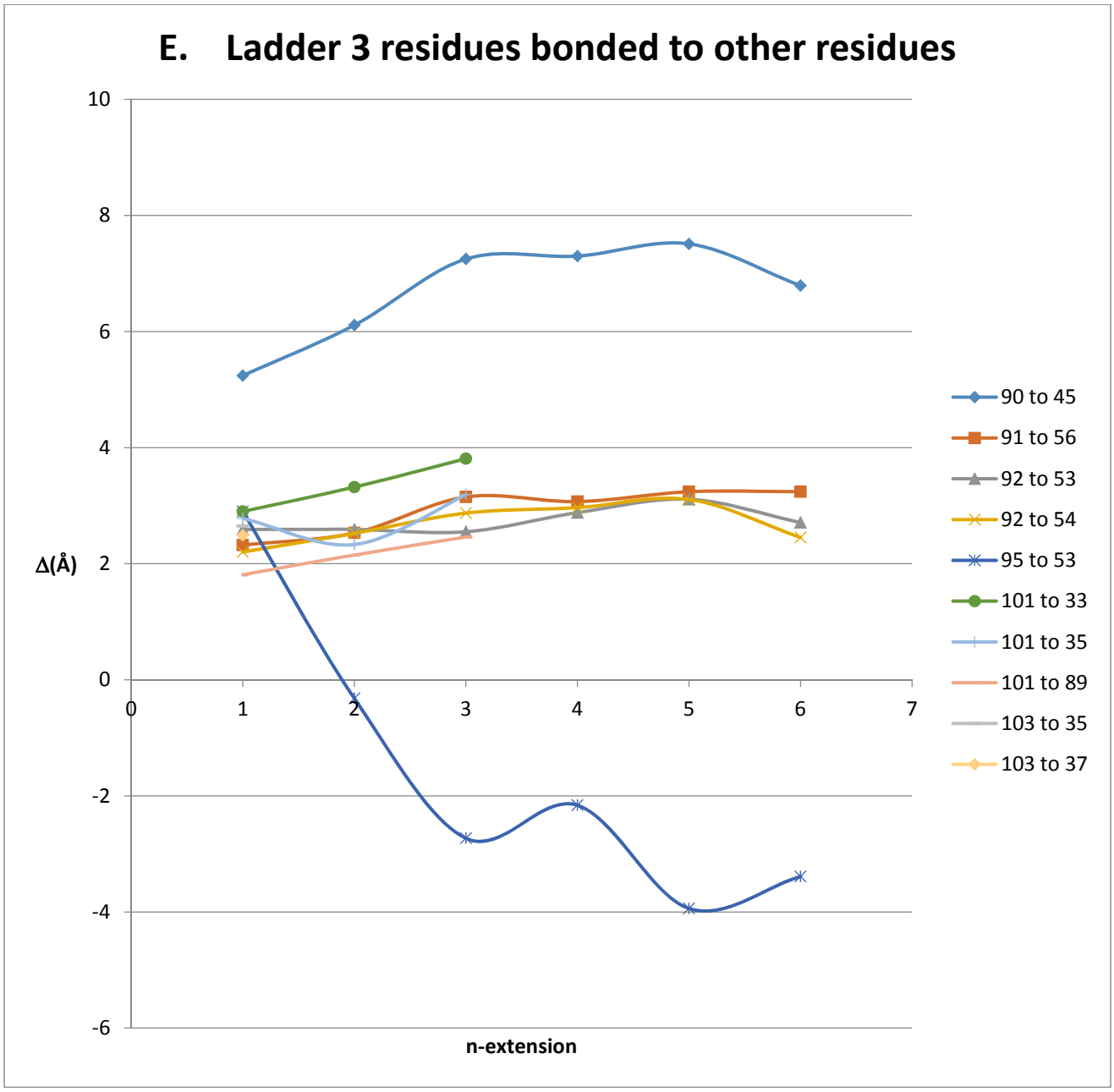

D. Ladder 3: Residues 86 to 92 bonded to Residues 95 to 104
6.00
5.00
4.00
3.00
2.00
1.00
0.00
-1.00
-2.00
-3.00
Δ(Å)
0
1
2
3
4
5
6
7
n-extension
88 to 102
88 to 84
89 to 101
90 to 100
91 to 99
92 to 98
95 to 98
95 to 92
96 to 99

Figure SI-5A


E. Ladder 3 residues bonded to other residues
10
8
6
4
2
0
-2
-4
-6
Δ(Å)
0
1
2
3
4
5
6
7
n-extension
90 to 45
91 to 56
92 to 53
92 to 54
95 to 53
101 to 33
101 to 35
101 to 89
103 to 35
103 to 37